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=> file registry

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FULL ESTIMATED COST 0.21 0.21

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http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\10613762_str.str

chain nodes : 10 11 12 19

ring nodes :

1 2 3 4 5 6 7 8 9 13 14 15 16 17 18

chain bonds :

7-10 9-11 11-12 12-13 16-19

ring bonds :

1-2 1-6 2-3 3-4 3-7 4-5 4-9 5-6 7-8 8-9 13-14 13-18 14-15 15-16 16-17 17-18

exact/norm bonds :

3-7 4-9 7-8 8-9

exact bonds :

7-10 9-11 11-12 12-13 16-19

normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 13-14 13-18 14-15 15-16 16-17 17-18

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS 11:CLASS 12:CLASS 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom 18:Atom 19:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 15:59:20 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 50 TO ITERATE

100.0% PROCESSED 50 ITERATIONS 2 ANSWERS

27 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 576 TO 1424

PROJECTED ITERATIONS: 576 TO 1424
PROJECTED ANSWERS: 2 TO 124

L2 2 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 15:59:24 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 905 TO ITERATE

100.0% PROCESSED 905 ITERATIONS

SEARCH TIME: 00.00.01

27 SEA SSS FUL L1

=> file medline, caplus, wpids, uspatfull

COST IN U.S. DOLLARS SINCE FILE TOTAL

> ENTRY SESSION

172.10 172.31 FULL ESTIMATED COST

FILE 'MEDLINE' ENTERED AT 15:59:33 ON 26 JAN 2007

FILE 'CAPLUS' ENTERED AT 15:59:33 ON 26 JAN 2007

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FILE 'USPATFULL' ENTERED AT 15:59:33 ON 26 JAN 2007

CA INDEXING COPYRIGHT (C) 2007 AMERICAN CHEMICAL SOCIETY (ACS)

=> s 13

SAMPLE SEARCH INITIATED 15:59:38 FILE 'WPIDS'

SAMPLE SCREEN SEARCH COMPLETED -1 TO ITERATE

100.0% PROCESSED 1 ITERATIONS O ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

> BATCH **COMPLETE**

PROJECTED ITERATIONS: 1 TO 40

PROJECTED ANSWERS: 0 TO

58 L3 T.4

=> s 14 not py>2001

16 L4 NOT PY>2001

=> d 15 1-16 ibib, abs, hitstr

ANSWER 1 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 2001:826093 CAPLUS Full-text

DOCUMENT NUMBER: 136:61809

TITLE: Indole- and carbazole-substituted pyridinium iodide

salts: a rare case of conformational isomerism in

crystals

Wang, Zheng; Nesterov, Vladimir N.; Borbulevych, Oleg AUTHOR (S):

Ya.; Clark, Ronald D.; Antipin, Mikhail Yu.;

Timofeeva, Tatiana V.

CORPORATE SOURCE: Department of Chemistry, New Mexico Highlands

University, Las Vegas, NM, 87701, USA

SOURCE: Acta Crystallographica, Section C: Crystal Structure

Communications (2001), C57(11), 1343-1348

CODEN: ACSCEE; ISSN: 0108-2701

PUBLISHER: Munksquard International Publishers Ltd.

DOCUMENT TYPE: Journal English LANGUAGE:

Indole- and carbazole-substituted pyridinium iodide salts were synthesized and AB characterized. X-ray anal. revealed that the iodide salt of the indolesubstituted cation (E)-4-(1H-indol-3-ylvinyl)-N-methylpyridinium (IMPE+), C16H15N2+·I-, (I), has two polymorphic modifications, (Ia) and (Ib), and a hemihydrate structure, C16H15N2+·I-·0.5H2O, (II). Until now, only one crystal modification was identified for the (E)-4-(9-ethyl-9H-carbazol-3-ylvinyl)-N-methylpyridinium (ECMPE+) iodide salt, C22H21N2+·I-, (III). Crystals of (Ia) and (Ib) comprise stacks of antiparallel cations with iodide anions located in the channels between the stacks. Due to the presence of the H2O mols., the packing in (II) is quite different to that found in (Ia) and (Ib), and positional disorder involving a statistical superposition of two rotamers of IMPE+, with different orientations of the indole fragment, was found. Crystals of (III) contain two independent ECMPE+ rotamers with different orientations of their carbazole substituents. The cations are packed in stacks, with the iodide anions located in the channels between the stacks. In (III), the iodide is disordered over two sites, with occupancies of 0.83 and 0.17. Crystallog. data are given.

IT 382591-35-7

RL: PRP (Properties)

(crystal structure of)

RN 382591-35-7 CAPLUS

CN Pyridinium, 4-[(1E)-2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide, hydrate (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 36098-33-6 CMF C16 H15 N2 . I

Double bond geometry as shown.

● I -

IT 36098-33-6P

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (preparation and crystal structure of polymorphs of)

RN 36098-33-6 CAPLUS

CN Pyridinium, 4-[(1E)-2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

REFERENCE COUNT:

24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L5 ANSWER 2 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1999:332021 CAPLUS Full-text

DOCUMENT NUMBER:

131:96967

TITLE:

Substituted 2- and 4-[2-(3-indoly1)ethenyl]pyridinium salts as inhibitors of MAO-B. Quantitative modeling of

the structure-activity relationship

AUTHOR (S):

Bachurin, S. O.; Fetison, V. I.; Afanas'ev, A. Z.; Afanas'eva, S. V.; Dubova, L. G.; Yankovskaya, V. L.;

Mukhina, T. V.

CORPORATE SOURCE:

Inst. Fiziol. Aktivnykh Veshchestv, Ross. Akad. Nauk,

Chernogolovka, Russia

SOURCE:

Doklady Akademii Nauk (1999), 364(6), 782-785

CODEN: DAKNEQ; ISSN: 0869-5652

PUBLISHER:

MAIK Nauka

DOCUMENT TYPE:

Journal

LANGUAGE:

Russian

AB Synthesis of 21 monoamineoxidase B inhibitors is reported. The modeling data demonstrate that combination of hydrophobic, polar, and steric factors dets. the degree of the enzyme inhibition.

IT 26608-75-3P 231954-87-3P 231955-03-6P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(substituted 2- and 4-[2-(3-indolyl)ethenyl]pyridinium salts as inhibitors of MAO-B: structure-activity relationship)

RN 26608-75-3 CAPLUS

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide (9CI) (CA INDEX NAME)

• I ·

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1,2,6-trimethyl-, iodide (9CI) (CA INDEX NAME)

• I •

RN 231955-03-6 CAPLUS

CN Quinolinium, 1-methyl-4-[2-(2-methyl-1H-indol-3-yl)ethenyl]-, iodide (9CI) (CA INDEX NAME)

• I -

L5 ANSWER 3 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1996:434896 CAPLUS Full-text

DOCUMENT NUMBER:

125:54703

TITLE:

Inhibition of dopamine reuptake system by analog of

neurotoxic metabolite MPP(1-methyl-4-

phenylpyridinium). Structure-activity relationships Bachurin, S. O.; Lukoyanov, N. V.; Petrova, L. N.;

Solyakov, L. S.; Tkachenko, S. E.; Raevskii, O. A.

CORPORATE SOURCE: Institut Fizi

Institut Fiziologicheski Aktivnykh Veshchestv,

Chernogolovka, Russia

SOURCE:

AUTHOR(S):

Doklady Akademii Nauk (1996), 346(4), 549-551

CODEN: DAKNEQ; ISSN: 0869-5652

PUBLISHER: MAIK Nauka
DOCUMENT TYPE: Journal
LANGUAGE: Russian

AB The quant. structure-activity anal. (QSAR) was carried out for 41 potential inhibitors of dopamine (I) reuptake of the series of 1-methyl-4-phenyl-1,2,3,4-tetrahydropyridine, 1-methyl-4-phenylpyridine, and stilbazole analogs. The structure-activity correlation equations were developed. QSAR demonstrated that the charge on the N atom of the pyridine cycle and hydrophilic substituents enhanced the inhibiting ability of the compds., while

the substituents more electroneg. than the N atom of the pyridine cycle caused a decrease in the affinity of the compds. to a I carrier.

IT 177997-46-5

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(QSAR study of inhibition of dopamine reuptake system by methylphenylpyridine analogs)

RN 177997-46-5 CAPLUS

CN Pyridinium, 1-methyl-4-[2-(2-methyl-1H-indol-3-yl)ethenyl]-, (E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

L5 . ANSWER 4 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1988:159032 CAPLUS Full-text

DOCUMENT NUMBER:

108:159032

TITLE:

Photolithographic material containing

contrast-enhancing layer

INVENTOR (S):

Ichimura, Kunihiro; Yonezawa, Teruhiko; Kikuchi,

Hideo; Tochizawa, Nariaki; Hayashi, Keiichi

PATENT ASSIGNEE(S):

Agency of Industrial Sciences and Technology, Japan;

Toyo Gosei Kogyo Co., Ltd.

SOURCE:

Eur. Pat. Appl., 31 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|------|----------|-----------------|-------------|
| | | | | |
| EP 246885 | A2 | 19871125 | EP 1987-304498 | 19870520 |
| EP 246885 | A3 | 19880622 | | |
| R: DE, FR, GB | | | | |
| JP 63100440 | Α | 19880502 | JP 1987-35781 | 19870220 |
| · JP 2592447 | B2 | 19970319 | | |
| JP 63100441 | Α | 19880502 | JP 1987-35782 | 19870220 |
| JP 2592448 | B2 | 19970319 | | |
| US 4925770 | Α | 19900515 | US 1988-284251 | 19881214 |
| PRIORITY APPLN. INFO.: | | | JP 1986-113508 | A 19860520 |
| | | | JP 1986-138144 | A 19860616 |
| | | | US 1987-47187 | B2 19870506 |

GI For diagram(s), see printed CA Issue.

AB A contrast-enhancing layer for a photolithog. material for formation of a patterned image (i.e., a resist image) by the light-projection method is comprised of a photobleachable compound having the structural unit represented by the formula I (Z = a divalent group which forms a heterocyclic aromatic ring structure with the N atom; X- = a monovalent anion; n = a pos. integer)

and a water-soluble polymer binder. Thus, a Si wafer was coated with a possworking photoresist composition (Microposit 1400-27), dried, overcoated with an aqueous solution containing II (a photobleachable compound) and pullulan, dried, exposed to UV (365 nm) radiation through a wafer stepper, and developed to give a line-and-space pattern (0.5 μ m width) with clear resolution

IT 113657-73-1

RL: USES (Uses)

(photobleachable contrast-enhancing layers containing, for photoresists)

RN 113657-73-1 CAPLUS

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 113657-72-0 CMF C16 H15 N2

$$CH$$
 CH N

CM 2

CRN 21228-90-0 CMF C H3 O4 S

Me-0-S03-

L5 ANSWER 5 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1981:103639 CAPLUS Full-text

DOCUMENT NUMBER: 94:103639

TITLE: Isolation and synthesis of 5-ethyl-2-methyl-11H-

pyrido[3,4-a]carbazolium hydroxide, a new indole

alkaloid type from Aspidosperma gilbertii

AUTHOR(S): Miranda, Edson Conde; Brieskorn, Carl Heinz; Blechert,

Siegfried

CORPORATE SOURCE: Inst. Pharm. Lebensmittelchem., Univ. Wuerzburg,

Wuerzburg, D-8700, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1980), 113(10), 3245-8

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal

LANGUAGE: German

GΙ

AB The indole alkaloid I was isolated from the bark of Aspidosperma gilbertii. I was synthesized by reaction of 3-indolecarboxaldehyde with 1-methyl-4propylpyridinium iodide to give II, which underwent photochem cyclization.

IT 76787-85-4P

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and photochem. cyclization of pyridocarbazol derivs. from)

RN76787-85-4 CAPLUS

Pyridinium, 4-[1-(1H-indol-3-ylmethylene)propyl]-1-methyl-, iodide (9CI) CN (CA INDEX NAME)

ANSWER 6 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER: 1981:64937 CAPLUS Full-text

DOCUMENT NUMBER: 94:64937

Vinylogous anhydro bases of pyridylindoles TITLE:

AUTHOR (S): Stupnikova, T. V.; Kalafat, V. N.; Klyuev, N. A.;

Marshtupa, V. P.; Sagitullin, R. S.

CORPORATE SOURCE: Donetsk. Gos. Univ., Donetsk, USSR

Khimiya Geterotsiklicheskikh Soedinenii (1980), (10), SOURCE:

1360-4

CODEN: KGSSAQ; ISSN: 0453-8234

DOCUMENT TYPE: Journal

LANGUAGE: Russian

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

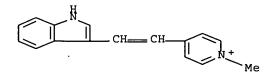
Treatment of I (R = Me, hexyl, dodecyl), II, and III with OH- gave IV (same AB R), V, and VI, resp., with little or no dealkylation. The pKa values of IV-VI were 10.00-11.17; protonation by HI occurred on the indolenine N atom to give the starting iodides. Alkylation and benzoylation of IV-VI also occurred on the indolenine N atom. IR, electronic, and mass spectral data were given for the anhydro bases.

26608-75-3 IT

> RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with hydroxide)

26608-75-3 CAPLUS RN

Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide (9CI) CN INDEX NAME)



I -

ANSWER 7 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1977:603333 CAPLUS Full-text

DOCUMENT NUMBER:

87:203333

TITLE:

Dyeing paper material

INVENTOR(S):

Moeckli, Peter

PATENT ASSIGNEE(S):

Ciba-Geigy A.-G., Switz.

SOURCE:

Ger. Offen., 23 pp. CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| TENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----------|--|--|--|--|
| 2711521 | A1 | 19770929 | DE 1977-2711521 | 19770316 |
| 2711521 | C3 | 19790201 | | |
| 601558 | A5 | 19780714 | CH 1976-3405 | 19760318 |
| 4089647 | Α | 19780516 | US 1977-767591 | 19770210 |
| 7700795 | Α | 19770919 | FI 1977-795 | 19770314 |
| 58532 | В | 19801031 | | |
| 58532 | C | 19810210 | | |
| 2344673 | A1 | 19771014 | FR 1977-7910 | 19770316 |
| 2344673 | B1 | 19800425 | | |
| 1107462 | A1 | 19810825 | CA 1977-274079 | 19770316 |
| 852553 | A1 | 19770919 | BE 1977-175853 | 19770317 |
| 7703056 | Α | 19770919 | SE 1977-3056 | 19770317 |
| 421077 | В | 19811123 | | |
| 421077 | C | 19820304 | | |
| 7701652 | Α | 19780103 | BR 1977-1652 | 19770317 |
| 456952 | A1 | 19780116 | ES 1977-456952 | 19770317 |
| 7701618 | Α | 19780222 . | ZA 1977-1618 | 19770317 |
| | TENT NO. 2711521 2711521 601558 4089647 7700795 58532 58532 2344673 2344673 1107462 852553 7703056 421077 421077 7701652 456952 7701618 | 2711521 A1 2711521 C3 601558 A5 4089647 A 7700795 A 58532 B 58532 C 2344673 A1 2344673 B1 1107462 A1 852553 A1 7703056 A 421077 B 421077 C 7701652 A 456952 A1 | 2711521 A1 19770929 2711521 C3 19790201 601558 A5 19780714 4089647 A 19780516 7700795 A 19770919 58532 B 19801031 58532 C 19810210 2344673 A1 19771014 2344673 B1 19800425 1107462 A1 19810825 852553 A1 19770919 7703056 A 19770919 421077 B 19811123 421077 C 19820304 7701652 A 19780103 456952 A1 19780116 | 2711521 A1 19770929 DE 1977-2711521 2711521 C3 19790201 601558 A5 19780714 CH 1976-3405 4089647 A 19780516 US 1977-767591 7700795 A 19770919 FI 1977-795 58532 B 19801031 58532 C 19810210 2344673 A1 19771014 FR 1977-7910 2344673 B1 19800425 1107462 A1 19810825 CA 1977-274079 852553 A1 19770919 BE 1977-175853 7703056 A 19770919 SE 1977-3056 421077 B 19811123 421077 C 19820304 7701652 A 19780103 BR 1977-1652 456952 A1 19780116 ES 1977-456952 |

| AU 7723350 | A | 19780921 | AU 1977-23350 | | 19770317 |
|------------------------|---|----------|---------------|---|----------|
| GB 1571927 | Α | 19800723 | GB 1977-11463 | | 19770317 |
| JP 54005002 | В | 19790313 | JP 1977-29359 | | 19770318 |
| PRIORITY APPLN. INFO.: | | | CH 1976-3405 | Α | 19760318 |

AB Addition of aqueous solns. of (indolylvinyl)-N-methylpyridinium chlorides to waste paper pulps gave colored papers. Thus, 50 g waste paper in 1 L H2O was beaten to obtain a fiber suspension, diluted with 1 L H2O, treated with 1 q 20% aqueous 1-methyl-2-[(2-methyl-1-H-indol-3-yl)vinyl]pyridinium chloride [64651-41-8] solution, diluted with H2O to 0.5% consistency, formed into paper web, and dried for 5 min at 100° to give waterproof, bright yellow wrapping paper.

64651-39-4P IT

RL: PREP (Preparation)

(dye for paper, manufacture of)

64651-39-4 CAPLUS RN

Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) CN INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & &$$

Cl -

ANSWER 8 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1972:69480 CAPLUS Full-text

DOCUMENT NUMBER:

76:69480

TITLE:

Inhibitors of choline acetyltransferase

AUTHOR (S):

Cavallito, C. J.; White, Helen Lyong; Yun, H. S.

CORPORATE SOURCE:

Sch. Pharm., Univ. North Carolina, Chapel Hill, NC,

SOURCE:

Drugs Cholinergic Mech. CNS (Cent. Nerv. Syst.), Proc.

Conf. (1970), 97-116. Editor(s): Heilbronn, Edith.

Foersvarets Forskningsanst.: Stockholm, Swed.

CODEN: 24HKAN

DOCUMENT TYPE:

Conference

LANGUAGE:

English

Choline acetyltransferase (ChAc) inhibitors were investigated. Results indicated that styrylpyridine derivs. and analogs are effective inhibitors. The structural and electronic features of the inhibitors are discussed. The inhibitors appear to block the transfer of acetyl from the acetyl CoA-ChAc complex to choline.

IT 36098-33-6

RL: BIOL (Biological study)

(choline acetyltransferase inhibition by)

36098-33-6 CAPLUS RN

CNPyridinium, 4-[(1E)-2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide (9CI) INDEX NAME)

Double bond geometry as shown.

OI.

ANSWER 9 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN

ACCESSION NUMBER:

1970:505755 CAPLUS Full-text

DOCUMENT NUMBER:

73:105755

TITLE:

Choline acetyltransferase inhibitors. Physicochemical

properties in relation to inhibitory activity of

styrylpyridine analogs

AUTHOR (S):

Allen, Richard Charles; Carlson, Gerald L.; Cavallito,

C. J.

CORPORATE SOURCE:

Sch. of Pharm., Univ. of North Carolina, Chapel Hill,

NC, USA

SOURCE:

Journal of Medicinal Chemistry (1970), 13(5), 909-12

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB Hueckel MO and Hansch calcns. were performed on various styrylpyridine derivs., some of which are potent inhibitors of choline acetyltransferase. These compds. apparently bind the enzyme by hydrophobic and π donor contributions of the aryl moiety, and π acceptor interactions, presumably by the pyridinium-like portion.

IT 29714-15-6

RL: PRP (Properties)

(mol. orbitals of, choline acetyltransferase inhibition in relation to)

RN 29714-15-6 CAPLUS

CN Pyridinium, 4-[(1E)-2-(1H-indol-3-yl)ethenyl]-1,3-dimethyl-, iodide (9CI) (CA INDEX NAME)

Double bond geometry as shown.

• I ·

L5 ANSWER 10 OF 16 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1970:107348 CAPLUS Full-text

DOCUMENT NUMBER:

72:107348

TITLE:

Choline acetyltransferase inhibitors. Dimensional and

substituent effects among styrylpyridine analogs

AUTHOR (S):

Cavallito, Chester J.; Yun, H. S.; Kaplan, T.; Smith,

John Crispin; Foldes, Francis F.

CORPORATE SOURCE:

Sch. of Pharm., Univ. of North Carolina, Chapel Hill,

NC, USA

SOURCE:

Journal of Medicinal Chemistry (1970), 13(2), 221-4

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Among styrylpyridine analogs, choline acetylase (ChA) inhibitory potency is diminished by highly electroneg. substituents (CN, NO2) on the 3- or 4-position of the phenyl ring but is enhanced by halogens (Cl, Br) less electroneg. than F. Substituents inducing deviation from coplanarity of the 2 ring systems are unfavorable for inhibitory activity. 3-Methyl substitution on the pyridine ring enhances potency. The nature of the pyrido-N-attached quaternizing group is noncritical and a hydrophilic substituent can provide potent, more water-soluble, derivs. A naphthyl vinyl-quinoline system provides a high order of potency, but the same mass distributed as in phenanthrylvinylpyridine is unfavorable. ChA inhibitory activity among these compds. seems favored by thin flat mols., one end of which tends to have π -electron-excessive, the other end π -electron-deficient, characteristics separated by a conjugating exocyclic bond. The photolability of some of these compds. in solution requires appropriate precautionary measures in their evaluation.

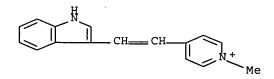
IT 26608-75-3

RL: BIOL (Biological study)

(choline acetyltransferase inhibition by)

RN 26608-75-3 CAPLUS

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, iodide (9CI) (CA INDEX NAME)



🗭 т -

L5 ANSWER 11 OF 16 USPATFULL on STN

ACCESSION NUMBER:

2001:66940 USPATFULL Full-text

TITLE:

Oxidation dyeing composition for keratin fibres and

dyeing method using said composition

INVENTOR (S):

de la Mettrie, Roland, Le Vesinet, France Cotteret, Jean, Verneuil-sur-Seine, France de Labbey, Arnaud, Aulnay Sous Bois, France

Maubru, Mireille, Chatou, France

PATENT ASSIGNEE(S):

L'Oreal S.A., Paris, France (non-U.S. corporation)

NUMBER KIND DATE

B1 PATENT INFORMATION: US 6228129 20010508

> WO 9917730 19990415

APPLICATION INFO.: US 1999-319166 19990701 (9) WO 1998-FR2075

> 19990701 PCT 371 date 19990701 PCT 102(e) date

19980928

DATE NUMBER

FR 1997-12353 PRIORITY INFORMATION: 19971003

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Liott, Caroline D.

Finnegan, Henderson, Farabow, Garrett & Dunner, L.L.P. LEGAL REPRESENTATIVE:

NUMBER OF CLAIMS: EXEMPLARY CLAIM: 1 LINE COUNT: 1560

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

The invention relates to a ready-to-use composition for the oxidation dyeing of keratin fibers, and in particular human keratin fibers such as the hair, comprising, in a medium which is suitable for dyeing, at least one oxidation base, at least one cationic direct dye and at least one enzyme of 2-electron oxidoreductase type in the presence of at least one donor for the said enzyme, and to the dyeing process using this composition.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

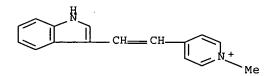
IT 64651-39-4

(oxidative hair dye compns. containing oxidoreductase-type enzymes, oxidation

bases, and direct cationic dyes)

RN 64651-39-4 USPATFULL

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) (CA



C1 -

ANSWER 12 OF 16 USPATFULL on STN L_5

1999:162994 USPATFULL Full-text ACCESSION NUMBER:

TITLE: Compositions and processes for dyeing keratin fibers

with cationic direct dyes, oxidation bases, and

oxidizing agents

Rondeau, Christine, Sartrouville, France INVENTOR (S):

Cotteret, Jean, Verneuil Sur Seine, France De La Mettrie, Roland, Le Vesinet, France

PATENT ASSIGNEE(S): L'Oreal, Paris, France (non-U.S. corporation) NUMBER KIND DATE

PATENT INFORMATION: US 6001135 19991214

APPLICATION INFO.: US 1997-994444 19971219 (8)

NUMBER DATE

PRIORITY INFORMATION: FR 1996-15895 19961223

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Liott, Caroline D.

LEGAL REPRESENTATIVE: Finnegan, Henderson, Farabow, Garrett & Dunner, L.L.P.

NUMBER OF CLAIMS: 41
EXEMPLARY CLAIM: 1
LINE COUNT: 823

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A ready-to-use composition for the oxidation dyeing of keratin fibers, in particular human keratin fibers such as the hair, this ready-to-use composition comprising at least one oxidation base in combination with at least one selected cationic direct dye and at least one oxidizing agent, as well as to the dyeing process using this ready-to-use composition.

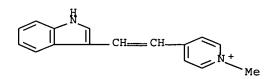
CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64651-39-4

(cationic direct colorant; oxidative hair dye compns. containing cationic direct colorants with good coloration, shine, and shampoo resistance)

RN 64651-39-4 USPATFULL

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)



● C1 -

L5 ANSWER 13 OF 16 USPATFULL on STN

ACCESSION NUMBER: 1999:154874 USPATFULL Full-text

TITLE: Composition for the oxidation dyeing of keratin fibers

containing a cationic direct dye and dyeing process

using this composition

INVENTOR(S): Rondeau, Christine, Sartrouville, France

Cotteret, Jean, Verneuil Sur Seine, France de la Mettrie, Roland, le Vesinet, France

PATENT ASSIGNEE(S): L'Oreal, France (non-U.S. corporation)

 NUMBER DATE

PRIORITY INFORMATION: FR 1996-15891 19961223

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Liott, Caroline D.

LEGAL REPRESENTATIVE: Finnegan, Henderson, Farabow, Garrett & Dunner, L.L.P.

NUMBER OF CLAIMS: 41
EXEMPLARY CLAIM: 1
LINE COUNT: 768

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

A ready-to-use composition for the oxidation dyeing of keratin fibers, in particular human keratin fibers such as the hair, comprising at least one oxidation base selected from para-phenylenediamines and bis(phenyl)alkylenediamines, in combination with at least one coupler selected from meta-diphenols, at least one selected cationic direct dye and at least one oxidizing agent, as well as to the dyeing process using this composition.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64651-39-4

(cationic direct dye; oxidative hair dye compns. with good coloration and shampoo resistance)

RN 64651-39-4 USPATFULL

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)

● C1 -

L5 ANSWER 14 OF 16 USPATFULL on STN

ACCESSION NUMBER: 1998:33383 USPATFULL Full-text

TITLE: Process for dyeing keratin-containing fibres with

cationic dyes

INVENTOR(S): Mockli, Peter, Sandgrubenstrasse, Switzerland

PATENT ASSIGNEE(S): Ciba Specialty Chemicals Corporation, Tarrytown, NY,

United States (U.S. corporation)

RELATED APPLN. INFO.: Continuation of Ser. No. US 1995-392783, filed on 28

Feb 1995, now abandoned

NUMBER DATE

PRIORITY INFORMATION: CH 1993-2020

19930705

DOCUMENT TYPE:

Utility

FILE SEGMENT:

Granted

PRIMARY EXAMINER:

Lieberman, Paul

ASSISTANT EXAMINER:

Dusheck, Caroline L.

LEGAL REPRESENTATIVE:

Mansfield, Kevin T.

NUMBER OF CLAIMS: EXEMPLARY CLAIM:

1

LINE COUNT:

691

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

Keratin-containing fibres, in particular human hair, are dyed using dyes of formulae (1) to (6) indicated in claim 1. These dyes make it possible to dye

by the trichromatic principle even in dark shades.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

64651-39-4

(hair dyeing prepns. containing cationic dyes)

64651-39-4 USPATFULL RN

Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) CN INDEX NAME)

$$CH$$
 CH
 CH
 N
 M
 M

ANSWER 15 OF 16 USPATFULL on STN

ACCESSION NUMBER:

90:38343 USPATFULL Full-text

TITLE:

Contrast-enhancing agent for photolithography

INVENTOR(S):

Ichimura, Kunihiro, Tsukuba, Japan Yonezawa, Teruhiko, Kanagawa, Japan

Kikuchi, Hideo, Chiba, Japan

Tochizawa, Nariaki, Funabashi, Japan Hayashi, Keiichi, Funabashi, Japan

PATENT ASSIGNEE(S):

Director General of Agency of Industrial Science and

Technology, Tokyo, Japan (non-U.S. government) Toyo Gosei Kogyo Co., Ltd., Chiba, Japan (non-U.S.

corporation)

NUMBER KIND

PATENT INFORMATION:

US 4925770

19900515

APPLICATION INFO.:

19881214 (7)

RELATED APPLN. INFO.:

US 1988-284251

Continuation-in-part of Ser. No. US 1987-47187, filed

on 6 May 1987, now abandoned

NUMBER DATE PRIORITY INFORMATION: JP 1986-113508 19860520

JP 1986-138144 19860616

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Michl, Paul R. ASSISTANT EXAMINER: Buscher, Mark R.

LEGAL REPRESENTATIVE: Hopgood, Calimafde, Kalil, Blaustein & Judlowe

NUMBER OF CLAIMS: 7
EXEMPLARY CLAIM: 1
LINE COUNT: 972

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

The invention provides a novel contrast-enhancing agent for photolithography which is used as an overcoating on a positive-working photoresist layer for enhancing the contrast of the photoresist in a low-contrast exposure to light. The composition comprises, in addition to a watersoluble polymer, e.g., poly(vinyl alcohol), poly(vinyl pyrroilidone) and pullulan, as the binder, a specific photo-bleachable organic compound having, in a molecule, at least one nitrogen-containing heterocyclic aromatic structure represented by the general formula ##STR1## in which Z is a divalent group to form the heterocyclic aromatic ring with the nitrogen atom, X is an anionic group of monovalency and n is a positive integer of, e.g., 1 or 2.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 113657-73-1

(photobleachable contrast-enhancing layers containing, for photoresists)

RN 113657-73-1 USPATFULL

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, methyl sulfate (9CI) (CA INDEX NAME)

CM 1

CRN 113657-72-0 CMF C16 H15 N2

$$CH$$
 CH
 CH
 N^+
 Me

CM 2

CRN 21228-90-0 CMF C H3 O4 S

Me-0-S03-

L5

ACCESSION NUMBER: 78:25171 USPATFULL Full-text

TITLE: Process for the dyeing of paper material

INVENTOR(S): Mockli, Peter, Basel, Switzerland

PATENT ASSIGNEE(S): Ciba-Geigy AG, Basel, Switzerland (non-U.S.

corporation)

NUMBER KIND DATE

PATENT INFORMATION: US 4089647 19780516

APPLICATION INFO.: US 1977-767591 19770210 (5)

NUMBER DATE

•-----

PRIORITY INFORMATION: CH 1976-3405 19760318

DOCUMENT TYPE: Utility FILE SEGMENT: Granted

PRIMARY EXAMINER: Schofer, Joseph L. ASSISTANT EXAMINER: Tungol, Maria S.

LEGAL REPRESENTATIVE: Roberts, Edward McC., Almaula, Probodh I.

NUMBER OF CLAIMS: 13
EXEMPLARY CLAIM: 1
LINE COUNT: 287

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

AB A process for the dyeing of paper material from an aqueous medium, comprising the use of at least one water-soluble dye of the formula ##STR1## wherein Py represents a pyridyl group of the formula ##STR2## R.sub.1 represents lower alkyl, substituted lower alkyl, allyl, or benzyl, R.sub.2 represents hydrogen, halogen, methyl or ethyl,

R.sub.3 represents hydrogen, methyl, ethyl or phenyl,

R.sub.4 represents hydrogen, lower alkyl substituted lower alkyl, or allyl, and

A.crclbar. represents an anion.

CAS INDEXING IS AVAILABLE FOR THIS PATENT.

IT 64651-39-4P

(dye for paper, manufacture of)

RN 64651-39-4 USPATFULL

CN Pyridinium, 4-[2-(1H-indol-3-yl)ethenyl]-1-methyl-, chloride (9CI) (CA INDEX NAME)

=> s 14 and "cell proliferation"

L6 1 L4 AND "CELL PROLIFERATION"

=> d 16 ibib, abs, hitstr

'HITSTR' IS NOT A VALID FORMAT FOR FILE 'MEDLINE'

ENTER DISPLAY FORMAT (BIB): ibib, abs

L6 ANSWER 1 OF 1 MEDLINE on STN

ACCESSION NUMBER: 2006351356 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 16766262

TITLE: Attenuation of LDH-A expression uncovers a link between

glycolysis, mitochondrial physiology, and tumor

maintenance.

AUTHOR: Fantin Valeria R; St-Pierre Julie; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard

Hughes Medical Institute, Boston, Massachusetts 02115, USA.

SOURCE: Cancer cell, (2006 Jun) Vol. 9, No. 6, pp. 425-34.

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200608

ENTRY DATE: Entered STN: 13 Jun 2006

Last Updated on STN: 10 Aug 2006

Entered Medline: 9 Aug 2006

AB Alterations in cellular metabolism are among the most consistent hallmarks of cancer. Herein we have investigated the relationship between increased aerobic lactate production and mitochondrial physiology in tumor cells. To diminish the ability of malignant cells to metabolize pyruvate to lactate, lactate dehydrogenase A (LDH-A) levels were knocked down by means of LDH-A short hairpin RNAs. Reduction in LDH-A activity resulted in stimulation of mitochondrial respiration and decrease of mitochondrial membrane potential. It also compromised the ability of these tumor cells to proliferate under hypoxia. The tumorigenicity of the LDH-A-deficient cells was severely diminished, and this phenotype was reversed by complementation with the human ortholog LDH-A protein. These results demonstrate that LDH-A plays a key role in tumor maintenance.

=> d his

(FILE 'HOME' ENTERED AT 15:58:45 ON 26 JAN 2007)

FILE 'REGISTRY' ENTERED AT 15:59:02 ON 26 JAN 2007

L1 STRUCTURE UPLOADED

L2 2 S L1

L3 27 S L1 FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 15:59:33 ON 26 JAN 2007

L4 58 S L3

L5 16 S L4 NOT PY>2001

L6 1 S L4 AND "CELL PROLIFERATION"

=> s 14 and "cancer"

L7 3 L4 AND "CANCER"

=> d 17 1-3 ibib, abs, hitstr

ENTER DISPLAY FORMAT (BIB): abs, ibib

L7 ANSWER 1 OF 3 MEDLINE on STN

AB Alterations in cellular metabolism are among the most consistent hallmarks of cancer. Herein we have investigated the relationship between increased aerobic lactate production and mitochondrial physiology in tumor cells. To diminish the ability of malignant cells to metabolize pyruvate to lactate, lactate dehydrogenase A (LDH-A) levels were knocked down by means of LDH-A short hairpin RNAs. Reduction in LDH-A activity resulted in stimulation of mitochondrial respiration and decrease of mitochondrial membrane potential. It also compromised the ability of these tumor cells to proliferate under hypoxia. The tumorigenicity of the LDH-A-deficient cells was severely diminished, and this phenotype was reversed by complementation with the human ortholog LDH-A protein. These results demonstrate that LDH-A plays a key role in tumor maintenance.

ACCESSION NUMBER: 2006351356 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 16766262

TITLE: Attenuation of LDH-A expression uncovers a link between

glycolysis, mitochondrial physiology, and tumor

maintenance.

AUTHOR: Fantin Valeria R; St-Pierre Julie; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard

Hughes Medical Institute, Boston, Massachusetts 02115, USA.

SOURCE: Cancer cell, (2006 Jun) Vol. 9, No. 6, pp. 425-34.

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200608

ENTRY DATE: Entered STN: 13 Jun 2006

Last Updated on STN: 10 Aug 2006 Entered Medline: 9 Aug 2006

L7 ANSWER 2 OF 3 MEDLINE on STN

Tumorigenesis results from events that impinge on a variety of collaborating metabolic pathways. To assess their role in this process, we utilized a cell-based assay to perform a high-throughput, chemical library screen. In so doing, we identified F16, a small molecule that selectively inhibits proliferation of mammary epithelial, neu-overexpressing cells, as well as a variety of mouse mammary tumor and human breast cancer cell lines. F16 belongs to a group of structurally similar molecules with a delocalized positive charge. The compound is accumulated in mitochondria of responsive cells, driven by the membrane potential, and it compromises their functional integrity. Mitochondrial hyperpolarization is a shared feature of many tumor cell lines, explaining the broad action spectrum of this novel delocalized lipophilic cation.

ACCESSION NUMBER: 2002401591 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 12150823

TITLE: A novel mitochondriotoxic small molecule that selectively

inhibits tumor cell growth.

AUTHOR: Fantin Valeria R; Berardi Marcelo J; Scorrano Luca;

Korsmeyer Stanley J; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School, Boston,

Massachusetts 02115, USA.

SOURCE: Cancer cell, (2002 Jul) Vol. 2, No. 1, pp. 29-42.

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200303

ENTRY DATE: Entered STN: 2 Aug 2002

Last Updated on STN: 26 Mar 2003 Entered Medline: 25 Mar 2003

L7 ANSWER 3 OF 3 MEDLINE on STN

AB Mitochondria are principal actors in apoptosis as central hubs for diverse apoptotic signals. A new paper demonstrates the therapeutic potential of directly engaging these apoptotic pathways by identifying a mitochondrial toxin selective for tumor cells.

ACCESSION NUMBER: 2002401587 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 12150816

TITLE: A mitochondrial Achilles' heel in cancer?.

AUTHOR: Hockenbery David M

CORPORATE SOURCE: Fred Hutchinson Cancer Research Center, Seattle, Washington

98109, USA.. dhockenb@fhcrc.rog

SOURCE: Cancer cell, (2002 Jul) Vol. 2, No. 1, pp. 1-2.

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY: United States

DOCUMENT TYPE: Commentary

Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200303

ENTRY DATE: Entered STN: 2 Aug 2002

Last Updated on STN: 26 Mar 2003 Entered Medline: 25 Mar 2003

=> d his

(FILE 'HOME' ENTERED AT 15:58:45 ON 26 JAN 2007)

FILE 'REGISTRY' ENTERED AT 15:59:02 ON 26 JAN 2007

L1 STRUCTURE UPLOADED

L2 2 S L1

L3 27 S L1 FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 15:59:33 ON 26 JAN 2007

L4 58 S L3

L5 16 S L4 NOT PY>2001

L6 1 S L4 AND "CELL PROLIFERATION"

L7 3 S L4 AND "CANCER"

---Logging off of STN---

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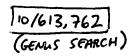
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Executing the logoff script...

=> LOG Y

| COST IN U.S. DOLLARS | SINCE FILE | TOTAL |
|--|------------|---------|
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 112.70 | 285.01 |
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| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -7.80 | -7.80 |

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COST IN U.S. DOLLARS

SINCE FILE TOTAL ENTRY SESSION 0.21 0.21

FULL ESTIMATED COST

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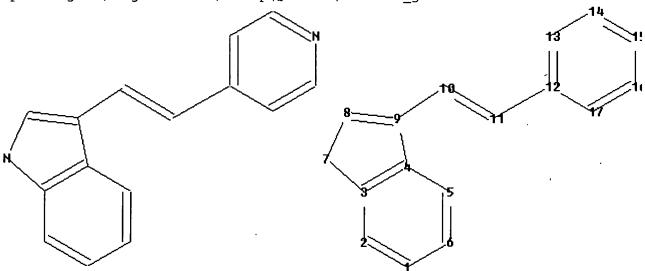
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http://www.cas.org/ONLINE/UG/regprops.html

Uploading C:\Program Files\Stnexp\Queries\10613762_genus.str



chain nodes :

10 11

ring nodes :

1 2 3 4 5 6 7 8 9 12 13 14 15 16 17

chain bonds :

9-10 10-11 11-12

ring bonds :

 $1-2 \quad 1-6 \quad 2-3 \quad 3-4 \quad 3-7 \quad 4-5 \quad 4-9 \quad 5-6 \quad 7-8 \quad 8-9 \quad 12-13 \quad 12-17 \quad 13-14 \quad 14-15 \quad 15-16$

16-17

exact/norm bonds:
3-7 4-9 7-8 8-9

exact bonds :

9-10 10-11 11-12 normalized bonds :

1-2 1-6 2-3 3-4 4-5 5-6 12-13 12-17 13-14 14-15 15-16 16-17

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:CLASS

11:CLASS 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:Atom

L1 STRUCTURE UPLOADED

=> d 11 .

L1 HAS NO ANSWERS

L1 STR

Structure attributes must be viewed using STN Express query preparation.

=> s 11

SAMPLE SEARCH INITIATED 16:07:16 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 313 TO ITERATE

100.0% PROCESSED 313 ITERATIONS

9 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 5199 TO 7321
PROJECTED ANSWERS: 9 TO 360

L2 9 SEA SSS SAM L1

=> s 11 full

FULL SEARCH INITIATED 16:07:20 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED - 6177 TO ITERATE

100.0% PROCESSED 6177 ITERATIONS 127 ANSWERS

SEARCH TIME: 00.00.01

L3 127 SEA SSS FUL L1

=> file medline, caplus, wpids, uspatfull

COST IN U.S. DOLLARS SINCE FILE TOTAL

ENTRY SESSION

FULL ESTIMATED COST 172.10 172.31

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FILE 'CAPLUS' ENTERED AT 16:07:29 ON 26 JAN 2007

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FILE 'USPATFULL' ENTERED AT 16:07:29 ON 26 JAN 2007

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=> s 13

SAMPLE SEARCH INITIATED 16:07:35 FILE 'WPIDS'

SAMPLE SCREEN SEARCH COMPLETED - 11 TO ITERATE

100.0% PROCESSED 11 ITERATIONS 0 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 11 TO 209

PROJECTED ANSWERS: 0 TO 0

L4 95 L3

=> s 14 and "cell proliferation"

L5 1 L4 AND "CELL PROLIFERATION"

=> d 15 ibib, abs

L5 ANSWER 1 OF 1 MEDLINE on STN

ACCESSION NUMBER: 2006351356 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 16766262

TITLE: Attenuation of LDH-A expression uncovers a link between

glycolysis, mitochondrial physiology, and tumor

maintenance.

AUTHOR: Fantin Valeria R; St-Pierre Julie; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard

Hughes Medical Institute, Boston, Massachusetts 02115, USA.

SOURCE: Cancer cell, (2006 Jun) Vol. 9, No. 6, pp. 425-34.

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200608

ENTRY DATE: Entered STN: 13 Jun 2006

Last Updated on STN: 10 Aug 2006

Entered Medline: 9 Aug 2006

AB Alterations in cellular metabolism are among the most consistent hallmarks of cancer. Herein we have investigated the relationship between increased aerobic lactate production and mitochondrial physiology in tumor cells. To diminish the ability of malignant cells to metabolize pyruvate to lactate, lactate dehydrogenase A (LDH-A) levels were knocked down by means of LDH-A short hairpin RNAs. Reduction in LDH-A activity resulted in stimulation of mitochondrial respiration and decrease of mitochondrial membrane potential. It also compromised the ability of these tumor cells to proliferate under hypoxia. The tumorigenicity of the LDH-A-deficient cells was severely diminished, and this phenotype was reversed by complementation with the human ortholog LDH-A protein. These results demonstrate that LDH-A plays a key role in tumor maintenance.

=> d his

(FILE 'HOME' ENTERED AT 16:06:43 ON 26 JAN 2007)

FILE 'REGISTRY' ENTERED AT 16:06:55 ON 26 JAN 2007

L1 STRUCTURE UPLOADED

L2 9 S L1

L3 127 S L1 FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 16:07:29 ON 26 JAN 2007

L4 95 S L3

L5 1 S L4 AND "CELL PROLIFERATION"

=> s 14 and "differentiation"

L6 0 L4 AND "DIFFERENTIATION"

=> s 14 and "tumor"

L7 5 L4 AND "TUMOR"

=> d 17 1-5 ibib, abs, hitstr

L7 ANSWER 1 OF 5 MEDLINE on STN

ACCESSION NUMBER: 2006351356 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 16766262

TITLE: Attenuation of LDH-A expression uncovers a link between

glycolysis, mitochondrial physiology, and tumor

maintenance.

AUTHOR: Fantin Valeria R; St-Pierre Julie; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard

Hughes Medical Institute, Boston, Massachusetts 02115, USA.

SOURCE: Cancer cell, (2006 Jun) Vol. 9, No. 6, pp. 425-34.

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200608

ENTRY DATE: Entered STN: 13 Jun 2006

Last Updated on STN: 10 Aug 2006

Entered Medline: 9 Aug 2006

AB Alterations in cellular metabolism are among the most consistent hallmarks of cancer. Herein we have investigated the relationship between increased aerobic lactate production and mitochondrial physiology in tumor cells. To diminish the ability of malignant cells to metabolize pyruvate to lactate, lactate dehydrogenase A (LDH-A) levels were knocked down by means of LDH-A short hairpin RNAs. Reduction in LDH-A activity resulted in stimulation of mitochondrial respiration and decrease of mitochondrial membrane potential. It also compromised the ability of these tumor cells to proliferate under hypoxia. The tumorigenicity of the LDH-A-deficient cells was severely diminished, and this phenotype was reversed by complementation with the human ortholog LDH-A protein. These results demonstrate that LDH-A plays a key role in tumor maintenance.

L7 ANSWER 2 OF 5 MEDLINE on STN

ACCESSION NUMBER: 2004029169 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 14729642

TITLE: F16, a mitochondriotoxic compound, triggers apoptosis or

necrosis depending on the genetic background of the target

carcinoma cell.

AUTHOR: Fantin Valeria R; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard

Hughes Medical Institute, Boston, Massachusetts 02115, USA.

SOURCE: Cancer research, (2004 Jan 1) Vol. 64, No. 1, pp. 329-36.

Journal code: 2984705R. ISSN: 0008-5472.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200404

ENTRY DATE: Entered STN: 21 Jan 2004

Last Updated on STN: 2 Apr 2004 Entered Medline: 1 Apr 2004

AΒ Mutations that lead to the emergence of resistance to apoptosis are commonly observed among tumor cells. Some of the proteins affected are integral parts of the apoptotic cascade such as pro- and antiapoptotic members of the Bcl-2 family. F16 is a small molecule that accumulates in mitochondria of a variety of tumor cells and interferes with their physiological function. Because this interference ultimately triggers apoptosis in many affected cell lines, we examined the effect of antiapoptotic Bcl-2 overexpression on the response of cells to F16. Our results showed that high levels of Bc1-2 did not block the ability of F16 to induce cell death. However, unlike the apoptotic response that followed F16 treatment of cells with moderate Bcl-2 levels, cells resistant to a variety of apoptotic stimuli by virtue of Bcl-2 overexpression succumbed to F16 by necrosis. Thus, this dual ability of the mitochondriotoxic compound F16 to induce apoptosis and necrosis may represent an added advantage by expanding its spectrum of action toward genetically altered tumor cells incapable of apoptosis.

L7 ANSWER 3 OF 5 MEDLINE on STN

ACCESSION NUMBER: 2002401591 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 12150823

TITLE: A novel mitochondriotoxic small molecule that selectively

inhibits tumor cell growth.

AUTHOR: Fantin Valeria R; Berardi Marcelo J; Scorrano Luca;

Korsmeyer Stanley J; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School, Boston,

Massachusetts 02115, USA.

SOURCE: Cancer cell, (2002 Jul) Vol. 2, No. 1, pp. 29-42.

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200303

ENTRY DATE: Entered STN: 2 Aug 2002

Last Updated on STN: 26 Mar 2003 Entered Medline: 25 Mar 2003

Tumorigenesis results from events that impinge on a variety of collaborating metabolic pathways. To assess their role in this process, we utilized a cell-based assay to perform a high-throughput, chemical library screen. In so doing, we identified F16, a small molecule that selectively inhibits proliferation of mammary epithelial, neu-overexpressing cells, as well as a variety of mouse mammary tumor and human breast cancer cell lines. F16 belongs to a group of structurally similar molecules with a delocalized positive charge. The compound is accumulated in mitochondria of responsive cells, driven by the membrane potential, and it compromises their functional integrity. Mitochondrial hyperpolarization is a shared feature of many tumor cell lines, explaining the broad action spectrum of this novel delocalized lipophilic cation.

L7 ANSWER 4 OF 5 MEDLINE on STN

ACCESSION NUMBER: 2002401587 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 12150816

TITLE: A mitochondrial Achilles' heel in cancer?.

AUTHOR: Hockenbery David M

CORPORATE SOURCE: Fred Hutchinson Cancer Research Center, Seattle, Washington

98109, USA.. dhockenb@fhcrc.rog

SOURCE: Cancer cell, (2002 Jul) Vol. 2, No. 1, pp. 1-2.

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY: United States

DOCUMENT TYPE: Commentary

Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200303

ENTRY DATE: Entered STN: 2 Aug 2002

Last Updated on STN: 26 Mar 2003 Entered Medline: 25 Mar 2003

AB Mitochondria are principal actors in apoptosis as central hubs for diverse apoptotic signals. A new paper demonstrates the therapeutic potential of directly engaging these apoptotic pathways by identifying a mitochondrial toxin selective for tumor cells.

L7 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2007 ACS on STN ACCESSION NUMBER: 1965:416812 CAPLUS Full-text

DOCUMENT NUMBER: 63:16812 ORIGINAL REFERENCE NO.: 63:2952a-b

TITLE: Styrylquinoline analogs from heterocyclic

carboxaldehydes

AUTHOR(S): Bahner, Carl Tabb; Kinder, Harold; Gutman, Lee

CORPORATE SOURCE: Carson-Newman Coll., Jefferson City, TN

SOURCE: Journal of Medicinal Chemistry (1965), 8(3), 397-8

CODEN: JMCMAR; ISSN: 0022-2623

DOCUMENT TYPE: Journal LANGUAGE: English

Indole-3-carboxaldehyde, pyridine-3-carboxaldehyde, thiophene-2-AB carboxaldehyde, and N-methyl-1,2,3,4-tetrahydroquinoline-6-carboxaldehyde were used to prepare a series of quinoline and isoquinoline derivs. which were studied for antitumor activity in relation to structure. 3-(3H-Indol-3ylidenemethyl)indole, 2-methyl-3- [(2-methyl-3H-indol-3- ylidene)methyl]indole, and 2-methyl-3-[1-(2-methyl-3H-indol-3-ylidene)- ethyl]indole showed greater antitumor activity against KB tumor cells than 2,2',2''methylidynetris[3-methylindole], 3,3',3''- methylidynetriindole, or 3,3',3''methylidynetris[2-methylindole]. The greater antitumor activity in the former group is believed to be due to the double bond joining the 2 ring systems. 1586-46-5P, Quinoline, 4-(2-indol-3-ylvinyl) - 1586-49-8P IT

, Quinoline, 4-[2-(1-methylindol-3-yl)vinyl]-

RL: PREP (Preparation)

(preparation of)

1586-46-5 CAPLUS RN

Quinoline, 4-(2-indol-3-ylvinyl)- (7CI, 8CI) (CA INDEX NAME) CN

1586-49-8 CAPLUS RN Quinoline, 4-[2-(1-methylindol-3-yl)vinyl]- (7CI, 8CI) (CA INDEX NAME) CN

=> d his

(FILE 'HOME' ENTERED AT 16:06:43 ON 26 JAN 2007)

FILE 'REGISTRY' ENTERED AT 16:06:55 ON 26 JAN 2007

Ll STRUCTURE UPLOADED

L29 S L1

L3 127 S L1 FULL FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 16:07:29 ON 26 JAN 2007

95 S L3 L4

1 S L4 AND "CELL PROLIFERATION" L5 0 S L4 AND "DIFFERENTIATION" L6

5 S L4 AND "TUMOR" L7

=> s 14 and cancer

3 L4 AND CANCER L8

=> d 18 1-3 ibib, abs, hitstr

'HITSTR' IS NOT A VALID FORMAT FOR FILE 'MEDLINE'

ENTER DISPLAY FORMAT (BIB): ibib, abs

ANSWER 1 OF 3 L8 MEDLINE on STN

ACCESSION NUMBER: 2006351356 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 16766262

TITLE: Attenuation of LDH-A expression uncovers a link between

glycolysis, mitochondrial physiology, and tumor

maintenance.

Fantin Valeria R; St-Pierre Julie; Leder Philip AUTHOR:

CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard Hughes Medical Institute, Boston, Massachusetts 02115, USA.

Cancer cell, (2006 Jun) Vol. 9, No. 6, pp. 425-34.

SOURCE:

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

200608 ENTRY MONTH:

ENTRY DATE: Entered STN: 13 Jun 2006

Last Updated on STN: 10 Aug 2006

Entered Medline: 9 Aug 2006

Alterations in cellular metabolism are among the most consistent hallmarks of AB cancer. Herein we have investigated the relationship between increased aerobic lactate production and mitochondrial physiology in tumor cells. diminish the ability of malignant cells to metabolize pyruvate to lactate, lactate dehydrogenase A (LDH-A) levels were knocked down by means of LDH-A short hairpin RNAs. Reduction in LDH-A activity resulted in stimulation of mitochondrial respiration and decrease of mitochondrial membrane potential. It also compromised the ability of these tumor cells to proliferate under hypoxia. The tumorigenicity of the LDH-A-deficient cells was severely diminished, and this phenotype was reversed by complementation with the human ortholog LDH-A protein. These results demonstrate that LDH-A plays a key role in tumor maintenance.

L8 ANSWER 2 OF 3 MEDLINE on STN

ACCESSION NUMBER: 2002401591 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 12150823

TITLE: A novel mitochondriotoxic small molecule that selectively

inhibits tumor cell growth.

AUTHOR: Fantin Valeria R; Berardi Marcelo J; Scorrano Luca;

Korsmeyer Stanley J; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School, Boston,

Massachusetts 02115, USA.

SOURCE: Cancer cell, (2002 Jul) Vol. 2, No. 1, pp. 29-42.

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY:

United States

DOCUMENT TYPE:

Journal; Article; (JOURNAL ARTICLE)

LANGUAGE:

English

FILE SEGMENT:

Priority Journals

ENTRY MONTH:

200303

ENTRY DATE:

Entered STN: 2 Aug 2002

Last Updated on STN: 26 Mar 2003 Entered Medline: 25 Mar 2003

Tumorigenesis results from events that impinge on a variety of collaborating metabolic pathways. To assess their role in this process, we utilized a cell-based assay to perform a high-throughput, chemical library screen. In so doing, we identified F16, a small molecule that selectively inhibits proliferation of mammary epithelial, neu-overexpressing cells, as well as a variety of mouse mammary tumor and human breast cancer cell lines. F16 belongs to a group of structurally similar molecules with a delocalized positive charge. The compound is accumulated in mitochondria of responsive cells, driven by the membrane potential, and it compromises their functional integrity. Mitochondrial hyperpolarization is a shared feature of many tumor cell lines, explaining the broad action spectrum of this novel delocalized lipophilic cation.

L8 ANSWER 3 OF 3

MEDLINE on STN

ACCESSION NUMBER:

2002401587 MEDLINE Full-text

DOCUMENT NUMBER:

PubMed ID: 12150816

TITLE:

A mitochondrial Achilles' heel in cancer?.

AUTHOR:

Hockenbery David M

CORPORATE SOURCE:

Fred Hutchinson Cancer Research Center, Seattle, Washington

98109, USA.. dhockenb@fhcrc.rog

SOURCE:

Cancer cell, (2002 Jul) Vol. 2, No. 1, pp. 1-2.

Journal code: 101130617. ISSN: 1535-6108.

PUB. COUNTRY:

United States

DOCUMENT TYPE:

Commentary
Journal; Article; (JOURNAL ARTICLE)

LANGUAGE:

English

FILE SEGMENT:

Priority Journals

ENTRY MONTH:

200303

ENTRY DATE:

Entered STN: 2 Aug 2002

Last Updated on STN: 26 Mar 2003 Entered Medline: 25 Mar 2003

AB Mitochondria are principal actors in apoptosis as central hubs for diverse apoptotic signals. A new paper demonstrates the therapeutic potential of directly engaging these apoptotic pathways by identifying a mitochondrial toxin selective for tumor cells.

=> d his

(FILE 'HOME' ENTERED AT 16:06:43 ON 26 JAN 2007)

FILE 'REGISTRY' ENTERED AT 16:06:55 ON 26 JAN 2007

L1 STRUCTURE UPLOADED

L2 9 S L1

L3 127 S L1 FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 16:07:29 ON 26 JAN 2007

L4 95 S L3

L5 1 S L4 AND "CELL PROLIFERATION"

L6 0 S L4 AND "DIFFERENTIATION"

L7 5 S L4 AND "TUMOR"

L8 3 S L4 AND CANCER

=> s 14 and "cell death"

L9 1 L4 AND "CELL DEATH"

=> d 19 ibib, abs

L9 ANSWER 1 OF 1 MEDLINE on STN

ACCESSION NUMBER: 2004029169 MEDLINE Full-text

DOCUMENT NUMBER: PubMed ID: 14729642

TITLE: F16, a mitochondriotoxic compound, triggers apoptosis or

necrosis depending on the genetic background of the target

carcinoma cell.

AUTHOR: Fantin Valeria R; Leder Philip

CORPORATE SOURCE: Department of Genetics, Harvard Medical School and Howard

Hughes Medical Institute, Boston, Massachusetts 02115, USA.

SOURCE: Cancer research, (2004 Jan 1) Vol. 64, No. 1, pp. 329-36.

Journal code: 2984705R. ISSN: 0008-5472.

PUB. COUNTRY: United States

DOCUMENT TYPE: Journal; Article; (JOURNAL ARTICLE)

LANGUAGE: English

FILE SEGMENT: Priority Journals

ENTRY MONTH: 200404

ENTRY DATE: Entered STN: 21 Jan 2004

Last Updated on STN: 2 Apr 2004 Entered Medline: 1 Apr 2004

AB Mutations that lead to the emergence of resistance to apoptosis are commonly observed among tumor cells. Some of the proteins affected are integral parts of the apoptotic cascade such as pro- and antiapoptotic members of the Bcl-2 family. F16 is a small molecule that accumulates in mitochondria of a variety of tumor cells and interferes with their physiological function. Because this interference ultimately triggers apoptosis in many affected cell lines, we examined the effect of antiapoptotic Bcl-2 overexpression on the response of cells to F16. Our results showed that high levels of Bcl-2 did not block the ability of F16 to induce cell death. However, unlike the apoptotic response that followed F16 treatment of cells with moderate Bc1-2 levels, cells resistant to a variety of apoptotic stimuli by virtue of Bcl-2 overexpression succumbed to F16 by necrosis. Thus, this dual ability of the mitochondriotoxic compound F16 to induce apoptosis and necrosis may represent an added advantage by expanding its spectrum of action toward genetically altered tumor cells incapable of apoptosis.

=> d his

(FILE 'HOME' ENTERED AT 16:06:43 ON 26 JAN 2007)

FILE 'REGISTRY' ENTERED AT 16:06:55 ON 26 JAN 2007

L1 STRUCTURE UPLOADED

L2 9 S L1

L3 127 S L1 FULL

FILE 'MEDLINE, CAPLUS, WPIDS, USPATFULL' ENTERED AT 16:07:29 ON 26 JAN 2007

L4 95 S L3

L5 1 S L4 AND "CELL PROLIFERATION"

L6 0 S L4 AND "DIFFERENTIATION"

=>

---Logging off of STN---

=>

Executing the logoff script...

=> LOG Y

| COST IN U.S. DOLLARS | SINCE FILE | $	exttt{TOTAL}$ |
|--|------------|-----------------|
| | ENTRY | SESSION |
| FULL ESTIMATED COST | 34.62 | 206.93 |
| | | |
| DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) | SINCE FILE | TOTAL |
| | ENTRY | SESSION |
| CA SUBSCRIBER PRICE | -0.78 | -0.78 |
| | | |

STN INTERNATIONAL LOGOFF AT 16:11:33 ON 26 JAN 2007